A Benchmark of Ubertally, MCNP, and SERA in a Full BNCT Source Optimization Study*

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Summary

A method of using a Monte Carlo code such as MCNP[1] to rapidly obtain multiple results for any number of different neutron sources transporting through identical geometries was developed at Lawrence Berkeley National Laboratories, known as the "Ubertally method." Preliminary studies[2] showed that this method could achieve statistically valid results in minutes compared to many hours when applied to a simple geometry such as a neutron source simulation through a head phantom. The results and efficiency of MCNP, SERA[3] and the "Ubertally method" were compared against each other in a full neutron beam optimization study. All three programs produced comparable results, strengthening the validity of our approach. The Ubertally program outperformed both SERA and MCNP in calculation speed, demonstrating its superiority in a multiple source theoretical study. SERA's calculation speed similarly outperformed MCNP, and is more useful in individual patient treatment planning than the Ubertally method, which can only be applied to constant-geometry simulations.

Introduction

The Ubertally method involves using MCNP in an initial simulation to record pertinent source and tally information for every particle that encounters a tally volume, such as a dose volume for a head phantom, in a single flat-spectrum, isotropic source. Results for a particular neutron

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or photon source are obtained by reading in this information and reweighting the tallied results to account for the new source, thus limiting the time-consuming head phantom particle transport to only a single initial simulation. To fully test this method's advantage and validity, a comparison was made using the Ubertally method in a complete neutron source optimization study versus performing the same study in MCNP or the treatment planning code SERA. In the same study, the SERA results could be compared independently against MCNP results. Hundreds of simulations were performed using each program, to determine the optimal moderator thickness for six different incident photon energies, from 2.1 MeV to 2.6 MeV on a ^{7}Li(p,n) neutron source, for three different moderators. Both the MCNP and SERA simulations were performed with 50 million neutrons and 50 million photons each. The "Ubertally method" was performed with 300 million neutrons and 300 million photons in the initial simulation. Users of the "Ubertally method," should keep in mind that the source will be biased to a logarithmically flat spectrum, with about 1% of the particles sampled in each 1/10th decade from thermal to 15.8 MeV. If the bulk of the particles in the thinnest spectrum to be simulated occupies only half of this range on a logarithmic scale, then twice the particles should be simulated to achieve equivalent results. By simulating 300 million particles, it is ensured that a spectrum as little as 1/6th the width of the range from thermal to 15.8 MeV may be simulated with equal confidence and that wider spectra will achieve even greater confidence for relatively minor increases in computer time.

Materials and Methods

A total of 248 simulations were performed using MCNP, SERA, and the "Ubertally method," modeling the same delimiter/phantom geometry but with 248 different neutron sources. The geometry consisted of a 20 cm diameter source channeled through a lithiated polyethylene delimiter which tapers the beam in a cone from 19 cm to a 12 cm aperture[4] before encountering an ellipsoidal modified Snyder head phantom[5,6] with brain, skull and scalp materials from ICRU46[7], with 10 ppm added ^{10}B. Each simulation actually consisted of two runs, modeling both neutrons and photon sources separately. These sources had been generated previously by 248 MCNP simulations of six different ^{7}Li(p,n) neutron source energies[8] through 12-17 thicknesses of the different moderators in a 25 cm diameter cylindrical geometry with an Al_2O_3 reflector.[9] The three moderators considered were a mixture of aluminum and aluminum flouride known as Fluental™,[10] enriched ^{7}LiF,[11] and heavy water. Dose rates were calculated along the beam centerline using standardized protocols and RBE values for BPA.[12] The therapeutic gain at brain midpoint (TG_{BM}) was used as a

figure of merit, defined as the ratio of the tumor dose at the center of the brain to the maximum tissue dose, within the constraints that the "entrance" dose be kept under 10 Gy-eq and treatment time for a 20 mA proton beam current be kept at approximately 1 hour or less. It was felt that keeping the entrance dose below 10 Gy-eq was necessary to ensure that the tissue depth-dose curve is rounded enough that the maximum tissue dose of 12.5 Gy-eq is contained within a relatively small volume.

Results

Tissue dose rates and its components along the beam centerline for one sample source are shown in Figure 1.

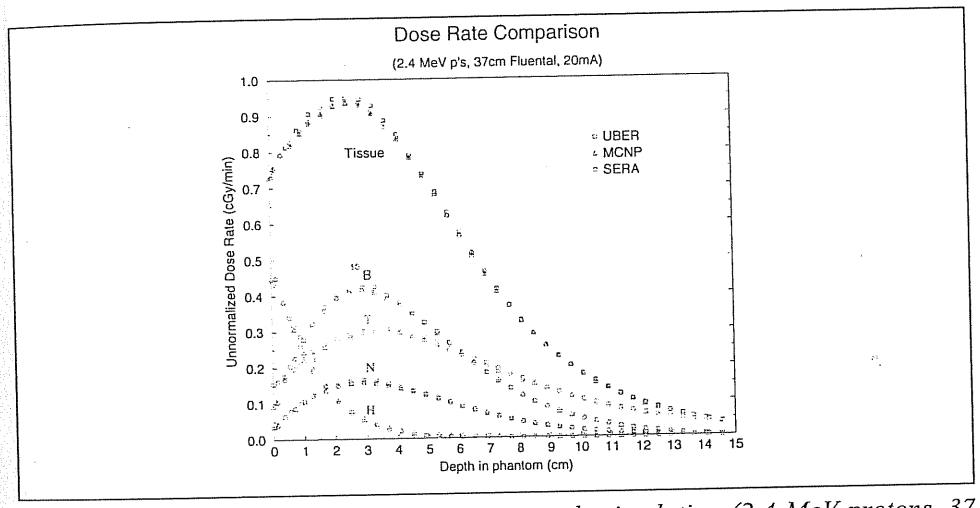

Figure 1 – Dose rate comparison for one example simulation (2.4 MeV protons, 37 cm Fluental). Error bars for MCNP and Ubertally are less than the dimensions of the datapoints. Uncertainty is not available for SERA.

Results from all three codes are included, along with a comparison of the difference in dose rates between MCNP and Ubertally for a similar case from a previous study in Figure 2. Error bars represent the square root of the sum of the squares of the relative uncertainties of the MCNP and Ubertally results, representing one standard deviation in the difference. Statistical theory states that 68% of the doses should lie within one standard deviation of each other. However, values in this study were often found to deviate significantly from simulation to simulation, as the datapoints within a single simulation are not statistically independent. Because SERA does not report statistical uncertainties in dose values, it was not possible to do a similar comparison. Results from 248 sets of data such as these, along with tumor dose curves, were used to determine

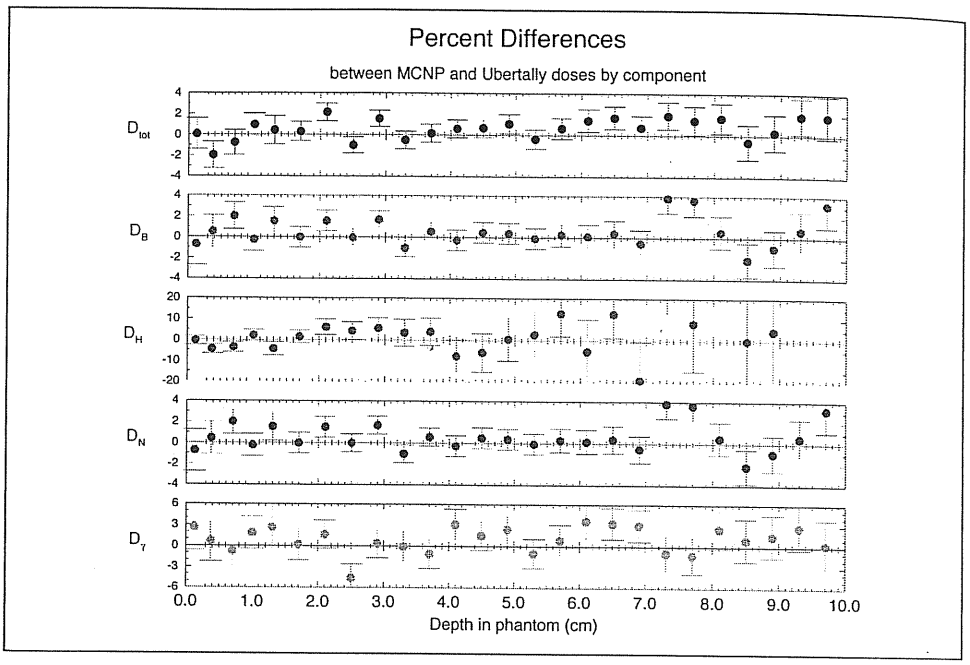

Figure 2 – Percent differences in dose rates in an example simulation (from a previous study) for the four tissue dose components and the total summed tissue dose. Error bars represent one standard deviation. Where the fast dose deviates significantly, dose is nearly zero and has little to no affect on total tissue dose.

optimal sources within the treatment parameters.

An example of the optimization of the thickness of Fluental for 2.5 MeV protons is shown in Figure 3. Each code predicts roughly the same thickness of moderator to produce the best neutron beam. Each code also predicts roughly the same neutron dose, within a degree of uncertainty, although SERA appears to predict slightly lower TG_{BM} values than MCNP and Ubertally. Graphs such as these were produced for all incident proton beam energies to produce the optimal designs shown in Table 1.

Table 1 – Doses are in Gy-eq

	MCNP	SERA	UBER
Moderator	Fluental	Fluental	Fluental
Proton Energy	2.5 MeV	2.4 MeV	2.5 MeV
Moderator thickness	39 cm	37 cm	39 cm
TG_{BM} (Brain Midpoint=7.3cm)	2.03(±.02)	1.98	2.01(±.01)
D_{tumor} @ B.M. (12.5 Gy-eq D_{tis})	25.4(±0.2)	24.8	25.2(±0.1)
Treatment Time (20 mA) [min]	72.7(±0.7)	65.8	72.1(±0.2)

Optimal advantage depths for ^{7}LiF ranged from 1.9 (SERA) to 1.94 (MCNP/UBER), at 51.3 minute and 40.7 minute treatment times,

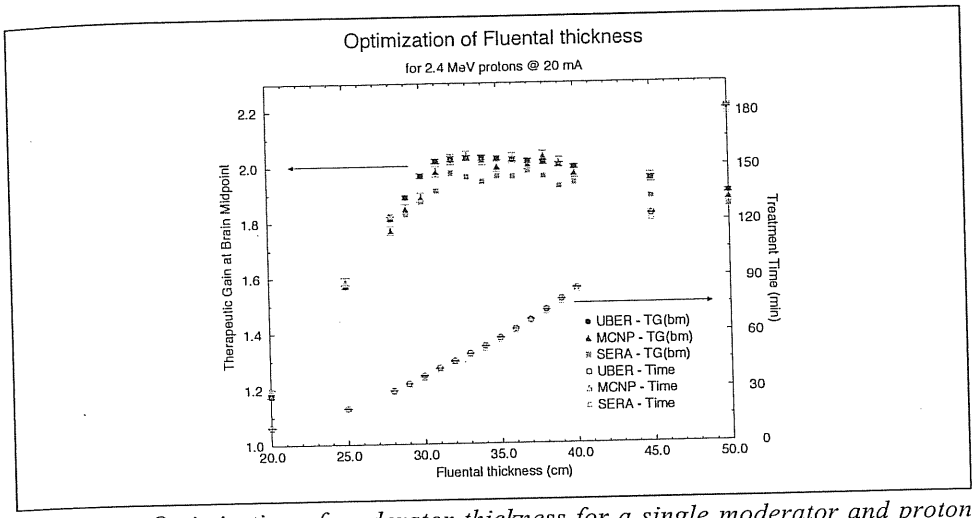

Figure 3 – Optimization of moderator thickness for a single moderator and proton energy, representing 17 simulations (out of 248). Thicknesses of less than 37 cm result in surface doses higher than 10 Gy-eq.

respectively. Optimal advantage depths for heavy water were generally less than 1.5 at comparable treatment time.

Figure 4 compares the computer time requirement to using each code, demonstrating the superiority of the Ubertally method when doing large-

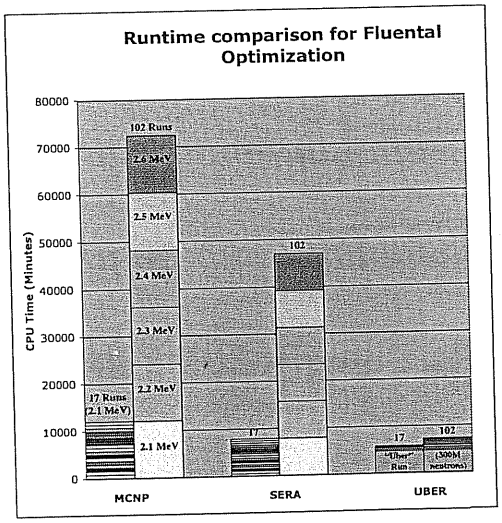

Figure 4 – Runtime Comparison of MCNP, SERA, and the "Ubertally method" for optimizing a single moderator, representing 102 of 248 runs). The first column shows individual simulations for one energy. The second column represents this optimization, plus six others. The bottom two blocks of the UBER column represent its one-time 300M particle simulation for photons (top) and neutrons (bottom).

scale optimization studies. The greater the number of same-geometry simulations that must be run, the greater is the advantage of this method.

While Ubertally has been shown to produce similar results to MCNP and SERA in a much shorter time, greater care must been taken to ensure the results are accurate. Figure 2 shows the statistical validity of a single Ubertally run. However, the dose points in that simulation are not statistically independent of each other. If the boron dose, for instance, is higher in one simulation than the other at a particular position in the head phantom, it is likely to also be higher at an adjacent position. The validity of the Ubertally method can be better evaluated by analyzing the difference in doses at a single position in the head phantom between MCNP and Ubertally for all 248 different neutron source simulations. This difference was divided by the sum of the squares of the relative uncertainties of each dose, producing a value representing the number of standard deviations away from agreement. Figure 5 is a histogram plot of these 248 values for the primary doses of interest, the boron dose at the brain midpoint and the total tissue dose at 2.5 cm, where it is most likely at a maximum for the best treatment beams. The distribution roughly follows statistical laws, which predict that 68% of the difference values should fall within one standard deviation, 95% within two, and 98% within three. This confirms that the doses produced by the Ubertally method are statistically accurate to within the reported uncertainties. However, an important feature to note is the apparent shift of the peak to negative values. This shift indicates that, on average, Ubertally produces slightly higher doses than MCNP, which is not readily apparent when comparing individual runs. Because Ubertally uses the same Monte Carlo simulation for every neutron source, each simulation is not statistically

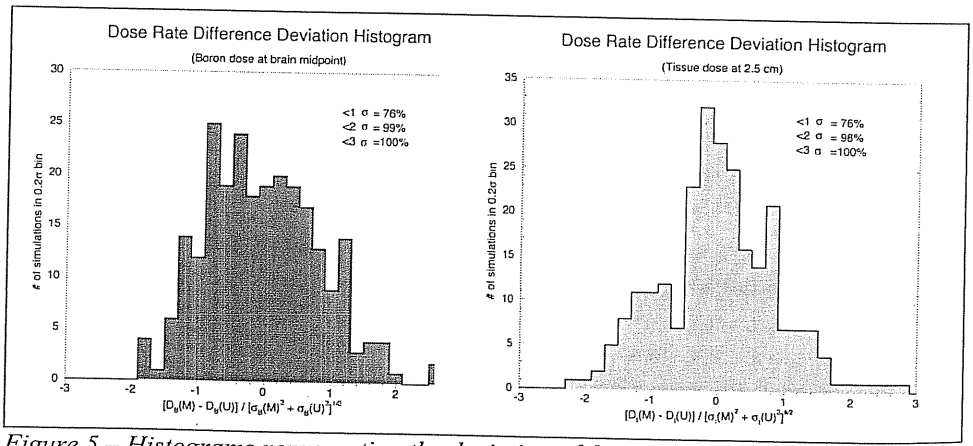

Figure 5 – Histograms representing the deviation of dose rate differences as a function of σ, the statistical uncertainty, for the important dose datapoints.

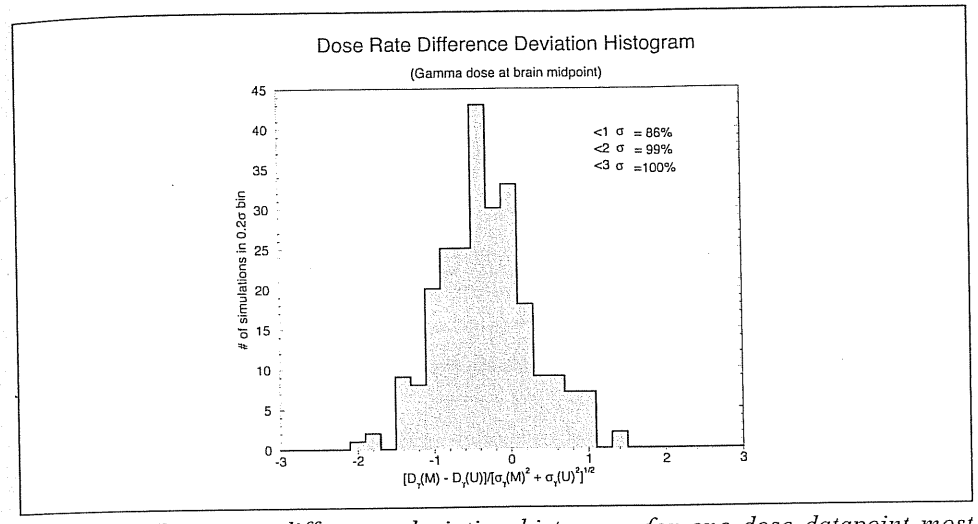

Figure 6 – Dose rate difference deviation histogram for one dose datapoint most seriously offset from the center, the gamma dose at the brain midp

independent. In large studies such as this, normal deviation from the actual answers will be systematic across all simulations. The effect is even more noticeable in specific doses and positions, such as the gamma dose at the brain midpoint seen in Figure 6, in which nearly 80% of the Ubertally doses are higher than those produced by statistically independent MCNP runs, instead of the 50% expected. The results are still applicable, as these deviations are normal to any Monte Carlo simulation and are represented in the relative uncertainties, well within a standard deviation. However, it is interesting to note that this analysis has shown more precisely the exact deviation of the Ubertally run and can therefore benefit from the many independent MCNP simulations to correct for its own statistical error. In effect, the actual statistical error becomes known to within far greater accuracy and can be accounted for, either with weighting factors or by analyzing new simulations with new random number seeds.

Conclusions/Summary

The Ubertally method has been shown to be a valuable tool in quickly performing optimization studies in which many different sources are considered transporting through a single geometry. In this example study, the savings in computer time was 16.5 times less than MCNP and 11 times less than SERA, while transporting six times as many particles. SERA was also shown to be a faster tool, taking 33% less computer time than MCNP. Because the Ubertally method is only applicable to same-geometry simulations, SERA is a more suitable tool for actual individual

treatment planning. The primary advantage to using MCNP over SERA is its uncertainty reporting and analysis.

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